

# Multicanonical hybrid Monte Carlo for compact QED

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We demonstrate that substantial progress can be achieved in the study of the phase structure of 4-dimensional compact QED by a joint use of hybrid Monte Carlo and multicanonical algorithms, through an efficient parallel implementation. This is borne out by the observation of considerable speedup of tunnelling between the metastable states, close to the phase transition, on the Wilson line. Our approach leads to a general parallelization scheme for the efficient stochastic sampling of systems where (a part of) the Hamiltonian involves the total action or energy in each update step.

## 1. Introduction

It is embarrassing that lattice simulations of compact QED still have not succeeded to clarify the order of the phase transition near  $\beta = 1$ , the existence of which was established in the classical paper of Guth [1]. This is mainly due to the failure of standard updating algorithms, like metropolis or heatbath to move the system at sufficient rate between the observed metastable states near its phase transition. Due to supercritical slowing down (SCSD) the tunneling rates decrease exponentially in  $L^3$  and exclude the use of lattices large enough to make contact with the thermodynamic limit by finite size scaling techniques (FSS) [2].

Torrie and Valleau [3] used arbitrary “non-physical” sampling distributions in their method, termed “umbrella sampling”, to improve the efficiency of stochastic sampling for situations when dynamically nearly disconnected parts of phase space occur by biasing the system to frequent the dynamically depleted, connecting regions of configuration space. Berg and Neuhaus [4] applied the idea of “umbrella sampling” under the name “multi-canonical algorithm” (MUCA) to the simulation of a variety of systems exhibiting first-order phase transitions. In this procedure, the biasing weight of a configuration with action  $S$  is dynamically adjusted such as to achieve a

near-constant overall frequency distribution over a wide range of  $S$  within a *single* simulation.

## 2. Multicanonical Sampling (MUCA)

“Canonical” Monte Carlo generates a sample of field configurations,  $\{\phi\}$  according to the Boltzmann weight  $P_{\text{can}}(\phi) \sim e^{-\beta S(\phi)}$ . The canonical action density which in general exhibits a double peak structure at a first-order phase transition, can be rewritten as

$$N_{\text{can}}(S, \beta) = \rho(S) e^{-\beta S}, \quad (1)$$

with the spectral density  $\rho(S)$  being independent of the inverse temperature  $\beta$ .

The multicanonical approach aims at generating a flat action density

$$N_{\text{MUCA}}(S, \beta_c) = \text{const.}, \text{ for } S_{\text{max1}} \leq S \leq S_{\text{max2}}, \quad (2)$$

in a range of  $S$  that covers the double peaks located at  $S_{\text{max1}}$  and  $S_{\text{max2}}$ . Therefore one modifies the sampling weights introducing a multicanonical potential  $V_{\text{MUCA}}(S)$ ,

$$P_{\text{MUCA}}(S) \sim e^{-\beta_c S - V_{\text{MUCA}}(S)}, \quad (3)$$

$$V_{\text{MUCA}}(S) = \begin{cases} \log N_{\text{can}}(S_{\text{max1}}, \beta_c) & S < S_{\text{max1}} \\ \log N_{\text{can}}(S, \beta_c) & S_{\text{max1}} \leq S \leq S_{\text{max2}} \\ \log N_{\text{can}}(S_{\text{max2}}, \beta_c) & S > S_{\text{max2}} \end{cases}$$

which is constant outside the relevant action range. Since  $V_{\text{MUCA}}(S)$  is unknown at the begin

of the simulation, it is instrumental for MUCA to bootstrap from good guesstimates. We shall do so by starting from an observed histogram of the canonical action density,  $\hat{N}_{\text{can}}(S, \hat{\beta}_c)$ , see eq. (1), at the supposed location of the phase transition,  $\hat{\beta}_c$ . From the action density, we compute  $\hat{V}_{\text{MUCA}}(S)$ . The sampling then proceeds with the full MUCA weight,

$$\begin{aligned} \hat{P}_{\text{MUCA}}(S) &\sim e^{-\hat{\beta}_c S - \hat{V}_{\text{MUCA}}(S)} \\ &\sim e^{-(\hat{\beta}_c + \hat{\beta}(S))S - \hat{\alpha}(S)}. \end{aligned} \quad (4)$$

In order to compute expectation values of observables, one has to reweight the resulting action density to reconstitute the proper canonical density  $P_{\text{can}}(S, \hat{\beta}_c) \sim \hat{P}_{\text{MUCA}}(S) e^{\hat{V}_{\text{MUCA}}(S)}$ . The computation of the multicanonical weights requires the knowledge of the global and not just the local change in action for each single update step. As a consequence, MUCA is not parallelizable for local update algorithms. For remedy, we propose to utilize the HMC updating procedure.

### 3. Hybrid Monte Carlo (HMC)

In addition to the gauge fields  $\phi_\mu(x)$  one introduces a set of statistically independent canonical momenta  $\pi_\mu(x)$ , chosen at random according to a Gaussian distribution  $\exp(-\frac{\pi_\mu^2}{2})$ . The action  $S[\phi]$  is extended to a guidance Hamiltonian

$$\mathcal{H}[\phi, \pi] = \frac{1}{2} \sum_{\mu, x} \pi_\mu^2(x) + \beta S[\phi]. \quad (5)$$

Starting with a configuration  $(\phi, \pi)$  at time  $t = 0$ , the system moves through phase space according to the equations of motion

$$\dot{\phi}_\mu = \frac{\partial \mathcal{H}}{\partial \pi_\mu} = \pi_\mu, \quad \dot{\pi}_\mu = -\frac{\partial \mathcal{H}}{\partial \phi_\mu} = -\frac{\partial}{\partial \phi_\mu}[\beta S], \quad (6)$$

leading to a proposal configuration  $(\phi', \pi')$  at time  $t = \tau$ . Finally this proposal is accepted in a global Metropolis step with probability

$$P_{\text{acc}} = \min(1, e^{-\Delta \mathcal{H}}), \quad \Delta \mathcal{H} = \mathcal{H}[\phi', \pi'] - \mathcal{H}[\phi, \pi]. \quad (7)$$

The equations of motion are integrated numerically with finite step size  $\Delta t$  along the trajectory from  $t = 0$  up to  $t = N_{\text{md}} \Delta t = \tau$ . Using the

leap-frog scheme [5] as symplectic integrator the discretized version of eq. (6) fulfills the *detailed balance* condition being time reversible and measure preserving. Each integration step approximates the correct  $\mathcal{H}$  with an error of  $O(\Delta t^3)$ .

### 4. Merging MUCA and HMC for Compact QED (MHMC)

We consider a multicanonical HMC for pure 4-dimensional  $U(1)$  gauge theory with standard Wilson action defined as

$$S[\phi] = \sum_{x, \nu > \mu} [1 - \cos(\theta_{\mu\nu}(x))],$$

$$\theta_{\mu\nu}(x) = \phi_\mu(x) + \phi_\nu(x + \hat{\mu}) - \phi_\mu(x + \hat{\nu}) - \phi_\nu(x).$$

Eq. 4 suggests to consider an *effective action*  $\hat{S}$  including the “multicanonical potential”  $V_{\text{MUCA}}$ ,

$$\hat{S} = \hat{\beta}_c S + \hat{V}_{\text{MUCA}}(S, \hat{\beta}_c) = (\hat{\beta}_c + \hat{\beta}(S))S + \hat{\alpha}(S). \quad (8)$$

We now define MHMC making use of the multicanonical potential as a driving term within molecular dynamics via the multicanonical Hamiltonian,  $\mathcal{H} = \frac{1}{2} \sum \pi^2 + \hat{S}$ , inducing an additional drift term such that the resulting force is given by

$$\dot{\pi}_\mu(x) = \left( \hat{\beta}_c + \hat{\beta}(S) \right) \sum_{\nu \neq \mu} \left[ \sin \theta_{\mu\nu}(x - \hat{\nu}) - \sin \theta_{\mu\nu}(x) \right]. \quad (9)$$

The MHMC is governed by the dynamics underlying the very two peak structure:  $V_{\text{MUCA}}$  is repelling the system out of the hot (cold) phase towards the cold (hot) phase, thus increasing its mobility and enhancing flip-flop activity<sup>1</sup>.

### 5. Tunneling Behaviour

In order to quantify the efficiency of the MHMC, we introduce the *average flip time*  $\tau_{\text{flip}}$  defined as the inverse number of the sum of flips between the two phases multiplied by the total number of trajectories. For reference, we additionally measured  $\tau_{\text{flip}}$  from the Metropolis algorithm with reflection steps (MRS) which is considered as a very effective local update algorithm for  $U(1)$  [7].

<sup>1</sup>Note that MHMC requires the computation of the global action (to adjust the correct multicanonical weight, eq. (4)) at each integration step along the trajectory of molecular dynamics to guarantee reversibility.

L	$\beta$	$\tau_{\text{flip}}^{\text{MRS}}$	$\tau_{\text{flip}}^{\text{MHMC}}$
6	1.001600	508(12)	650(20)
8	1.007370	1023(60)	1173(50)
10	1.009300	2474(117)	2006(84)
12	1.010143	5470(770)	3260(440)
14	1.010668	16400(3300)	5090(630)
16	1.010753	44800(9700)	6350(860)

$\tau_{\text{flip}}$  for the various lattices of volume  $V = L^4$ .

With the results for  $\tau_{\text{flip}}$  on lattices up to  $16^4$  we are in the position to estimate the scaling behaviour of MHMC in comparison to standard MRS updates. According to the expected exponential behaviour of  $\tau_{\text{flip}}^{\text{MRS}}$  which, in the asymptotic regime  $L \rightarrow \infty$ , should be given by  $\tau_{\text{SCSD}} \sim \exp(2\sigma L^3)$ , we perform a  $\chi^2$ -fit with the ansatz:

$$\tau_{\text{flip}}^{\text{MRS}} = a L^b e^{cL^3}. \quad (10)$$

which yields  $\chi_{\text{per d.o.f.}}^2 = 0.897$ . As a result, we find a clear exponential SCSD behaviour for the MRS algorithm. On the other hand, for the tunneling times of the MHMC, we expect a monomial dependence in  $L$ :

$$\tau_{\text{flip}}^{\text{MHMC}} = p L^q \quad (11)$$

The power law ansatz is well confirmed by the fit quality with  $\chi_{\text{per d.o.f.}}^2 = 0.795$ . We also took the pessimistic ansatz and tried to detect a potentially exponential increase of  $\tau_{\text{flip}}^{\text{MHMC}}$ . The exponential fit gives  $\chi_{\text{per d.o.f.}}^2 = 0.975$ .

[width=7.5cm]tflopprognose.obj.eps

Sustained CPU time in Tflop-hours to generate one flip based on tunneling times for MRS (exponential fit) and MHMC (lower curve is power law, upper curve is exponential fit). The errors of the two exponential fits are depicted as dotted lines. The error of the power law fit is not visible on this scale.

In order to compare the efficiency we have to take into account the computational effort. The complexity of the local Metropolis is given by  $t_{\text{MRS}} \sim V$  whereas the optimized leapfrog scheme in MHMC scales as  $t_{\text{MHMC}} \sim V^{5/4}$  [8]. As can be seen in the upper figure, the exponential contribution remains suppressed in the extrapolation. A potentially dominating exponential behaviour for MHMC can only be detected in future MHMC simulations on larger lattices.

## 6. Conclusions

We proposed to make use of the multicanonical (MUCA) algorithm within the hybrid Monte Carlo (HMC) updating scheme in order to boost the tunneling rates. Since both algorithms are inherently of global nature, their combination allows the parallelization of MUCA which could not be achieved otherwise. We have demonstrated that the fully parallel MHMC algorithm is capable to overcome SCSD in compact QED in practical simulations, at least up to lattices sizes  $\approx 24^4$ . On a  $24^4$  lattice we predict a gain factor of about 1000 for MHMC over the local metropolis algorithm with additional reflection. So far, we have encouraging experiences on the  $18^4$  lattice well confirming the extrapolations. The investigations presented form part of an ongoing study that aims at a conclusive FSS analysis of compact QED on the Wilson line [6].

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